2,3-Dihydroxynaphthalene 92-44-4 | DTXSID2043903

Model Performance

Model	Data	
Model	Dala	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 7.97

Global applicability domain: Outside

Local applicability domain index: 2.55e-01

Confidence level: 3.67e-01

Nearest Neighbors from the Training Set

Image not found

4-Hydroxybenzoic acid

Measured: 8.08 Predicted: 7.78

Image not found

Salicylic acid

Measured: 7.44 Predicted: 7.60

Image not found

Phenacetin

Measured: 9.59 **Predicted:** 9.23

Image not found

Diphenylamine Measured: 7.64 Predicted: 8.73 Image not found

Methylparaben Measured: 8.57 Predicted: 7.06